DERIVING STRUCTURAL ISOMERS OF STRAIGHT CHAIN ALKANES

Alfred Addo-Yobo © 2014

Abstract:

Identifying structural isomers of straight chain alkanes isn't as easy as it may require thorough check up, drawing of structures, double checking position of substituents on specific carbon atoms, etc. This process may be tedious, cumbersome as well as time consuming. In this paper, we shall present a new module for listing structural isomers of straight chain alkanes through the introduction of three power rules. These rules would serve as basis to also validate a compound as a structural isomer of a particular straight chain alkane or not.

Keywords: Straight chain alkanes, structural isomers, rules, carbon atoms, substituent

Introduction:

The module to be discussed is valid for structural isomers containing only methyl groups as substituents. The rules to be introduced will enable anyone to spot permissible or non-permissible structural isomers of a particular straight chain alkane. In order for a compound to pass for a structural isomer of a particular straight chain alkane, it must not contradict any of the rules to be introduced.

Addo-Yobo's rules of structural isomers

Rule 1:

The limit to single number locant numbers of structural isomers is n/2 for even carbon number straight chain alkanes and ½ (n – 1) for odd carbon number straight chain alkanes where n is the number of carbon atoms in the straight chain alkane.

Some structural isomers consists of two or three locant numbers such as 2, 3 dimethylbutane and 2,2,3 trimethyl pentane respectively. Other structural isomers contain only one locant number such as 2 methyl propane. What rule 1 states is that, single locant numbers of structural isomers of a particular straight chain alkanes has a limit. Consider the straight chain alkane, heptane. It's possible to have a blend of single, double and even triple digit locant numbers of structural isomers of this alkane. According to rule 1, the limit to single digit locant number structural isomers of this alkane is *½ (n – 1)* since it has an odd carbon number. This implies that the limit of single digit locant number will be ½ (7 – 1) = 3. Since the value is 3, it means that the only single digit locant number structural isomers of heptane possible are 2 methyl hexane and 3 methyl hexane. This further implies that a 4 methyl hexane and beyond is impossible.

NB: The rules are valid for structural isomers with methyl groups as the only substituents.

Rule 2:

No locant number in a structural isomer must correspond to or be greater than the carbon number of alkane in the structural isomer.

According to rule 2, it's impossible to have compounds such as 2,2,3 trimethylpropane and 2, 4 dimethyl butane as valid not to talk of them being structural isomers. This is because, the former has the number 3 as locant number, corresponding to the carbon number of alkane in the isomer which is propane. The latter also has a locant number 4 which corresponds to the carbon number of alkane in the isomer which is butane.

Rule 3:

For structural isomers with only two locant numbers, both number must not sum up to the carbon number of parent straight chain alkane carbon number.

This rule implies that considering the straight chain alkane hexane for example, it's impossible to have the following as structural isomers of hexane;

2, 4 dimethylbutane and 3, 3 dimethylbutane. This is because, both compounds consists of only two locant numbers which sum up to the carbon number (6) of parent straight chain alkane, hexane.

These are the underlying rules for validating all structural isomers of any straight chain alkane with methyl groups as the only substituents. ***If any structural isomers with methyl groups as the only substituents breaks any of the three rules, it does not qualify as a structural isomer of the straight chain alkane under consideration.***

Since the three rules of structural isomers have been introduced, we shall now discuss how to easily list all possible structural isomers of straight chain alkanes with methyl groups as the only substituents.

NEW MODULE FOR DERIVING STRUCTURAL ISOMERS

The characteristic feature of structural isomers that needs specific caution is the combination of locant numbers. When these combinations are wrong, the structural isomer becomes invalid. In this module, we are going to discuss a method by which all possible locant numbers of structural isomers can be derived and then the three rules introduced above will help eliminate the invalid isomers leaving us with permissible structural isomers.

NB: Once again, this module is valid only for structural isomers with methyl groups as the substituents.

In a problem where a student is required to list possible structural isomers of a particular straight chain alkane, the carbon number of the alkane under consideration must be known… For purposes of a quick example, let's consider the straight chain alkane, hexane.

It must be known that hexane has a carbon number of six. The next step in the module is to list the numbers from 2, 3….n where n is the carbon number of straight chain alkane under consideration and in this case, 6. Therefore, our list of numbers will be 2, 3, 4, 5, 6.

After this list is derived, the possible locant numbers of the structural isomers can be derived. ***The possible locant numbers of structural isomers are all possible combination of numbers that sum up to each of the numbers on the list.***

Two key points must also be noted;

1. In writing structural isomers of straight chain alkanes, the number one (1) cannot be a possible locant number.
2. No number can appear more than twice as possible locant number. This means, it's impossible to have say, 2, 2, 2 trimethyl pentane…

Let's now take each number on the list above and find all possible combination of numbers that sum up to each number on the list which is 2, 3, 4, 5, 6

NUMBERS	**ALL POSSIBLE COMBINATIONS THAT SUM UP**
2	(2)
3	(3)
4	(4), (2, 2)
5	(5), (2, 3)
6	(6), (3, 3), (2, 4)

From the possible combinations above, we can see there are single digit locant numbers 2, 3, 4, 5, 6 as well as double locant numbers which are (2, 2), (2, 3), (3, 3), (2, 4). These combinations make up the possible locant numbers of structural isomers for the straight chain alkane, hexane. Thus, we can go on to list the possible structural isomers as;

- 2 methyl pentane…… (1)
- 3 methyl pentane…… (2)
- 4 methyl pentane…… (3)
- 2, 2 dimethyl butane……... (4)
- 5 methyl pentane……. (5)
- 2, 3 dimethyl butane…… (6)
- 6 methyl pentane…….. (7)
- 3, 3 dimethyl butane……. (8)
- 2, 4 dimethyl butane……. (9)

The above are possible structural isomers of hexane. However, the rules earlier introduced shall be applied to eliminate the non-permissible structural isomers. Any of the above that contradicts any of the three rules becomes invalid as a structural isomer.

Let's first deal with the single digit locant numbers which is explicitly described by rule 1.

The limit to single number locant numbers of structural isomers is n/2 for even carbon number straight chain alkanes and ½ (n – 1) for odd carbon number straight chain alkanes where n is the number of carbon atoms in the straight chain alkane.

Since the straight chain alkane under consideration is hexane with an even carbon number of six, the limit to its single digit locant number structural isomer is n/2 = 6/2 = 3. This means that any single digit locant number structural isomer greater than 3 is invalid. This rule thus eliminates equations (3), (5), (7).

For the double digit locant number structural isomers, rules 2 and 3 apply. Equations (4) and (5) do not contradicts any of the rules thus considered valid. However, equation (8) and (9)

contradicts rule 3 since the structural isomer consists of only two locant numbers which sum up to the carbon number of parent straight chain alkane (hexane). This implies that the permissible structural isomers of hexane with only methyl groups as substituents are **2 methyl pentane, 3 methyl pentane, 2, 2 dimethyl butane** and **2, 3 dimethyl butane.**

In the event of any other straight chain alkane, the same rules and procedure must be applied to reveal all permissible structural isomers of straight chain alkanes with methyl groups as the only substituents.

Procedure:

- List the numbers from 2, 3… n where n is the carbon number of straight chain alkane under consideration
- Find all possible combination of numbers that sum up to each of the number on the list.
- The three rules earlier introduced will be employed to eliminate all invalid structural isomers.

NB: Always remember that there are cases where in the event of the number seven (7) in the list of numbers, possible number combinations that sum up to seven are (3, 4), (2, 5), (2, 2, 3). The key is to exhaust all possible combination of numbers that sum up to each number on the list. It's thus possible to have a three or four digit locant number structural isomer.